

10518612

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 09:21:14 ON 11 JUN 2007

FILE 'REGISTRY' ENTERED AT 09:21:41 ON 11 JUN 2007  
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**STRUCTURE FILE UPDATES:** 10 JUN 2007 **HIGHEST RN** 936909-28-3  
**DICTIONARY FILE UPDATES:** 10 JUN 2007 **HIGHEST RN** 936909-28-3

New CAS Information Use Policies. enter HELP USAGETERMS for details.

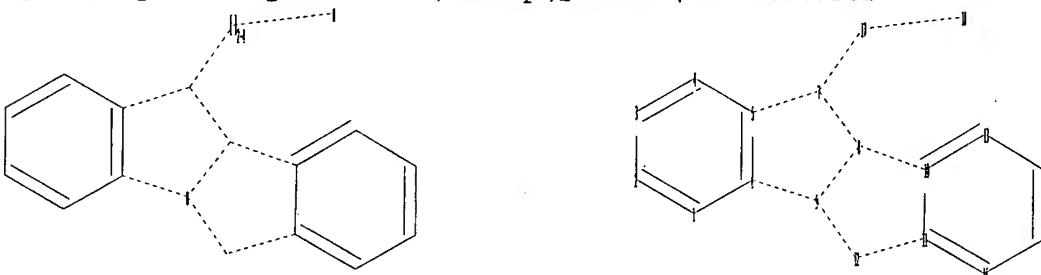
TSCA INFORMATION NOW CURRENT THROUGH December 3, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stn/gen/stndoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10518612.str



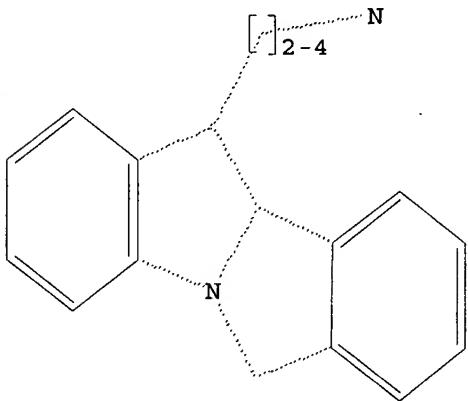
10518612

chain nodes :  
17 18  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16  
chain bonds :  
7-17 17-18  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-10 9-12 10-11 10-13 11-12  
11-16 13-14 14-15 15-16  
exact/norm bonds :  
5-7 6-9 7-8 7-17 8-9 8-10 9-12 11-12 17-18  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-13 11-16 13-14 14-15 15-16

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L1 STRUCTURE UPLOADED

=> D  
L1 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1  
SAMPLE SEARCH INITIATED 09:22:14 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 120 TO ITERATE

100.0% PROCESSED 120 ITERATIONS 5 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1743 TO 3057  
PROJECTED ANSWERS: 5 TO 234

10518612

L2 5 SEA SSS SAM L1

=> S L1 FULL  
FULL SEARCH INITIATED 09:22:20 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 2433 TO ITERATE

100.0% PROCESSED 2433 ITERATIONS 106 ANSWERS  
SEARCH TIME: 00.00.01

L3 106 SEA SSS FUL L1

=> FILE CAPLUS  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
172.10 172.31

FILE 'CAPLUS' ENTERED AT 09:22:26 ON 11 JUN 2007  
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FILE COVERS 1907 - 11 Jun 2007 VOL 146 ISS 25  
FILE LAST UPDATED: 10 Jun 2007 (20070610/ED)

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=> S L3  
L4 12 L3

=> D IBIB ABS HITSTR TOT

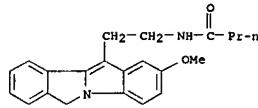
10518612

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:1177614 CAPLUS  
 DOCUMENT NUMBER: 146:55814  
 TITLE: Differences in binding sites of two melatonin receptors help to explain their selectivity to some melatonin analogs: a molecular modeling study  
 AUTHOR(S): Chugunov, Anton O.; Farce, Amaury; Chavatte, Philippe;  
 CORPORATE SOURCE: Efremov, Roman G.  
 Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, GSP Moscow, 117997, Russia  
 SOURCE: Journal of Biomolecular Structure and Dynamics (2006), 24(2), 91-107  
 PUBLISHER: Adenine Press  
 DOCUMENT TYPE: CODEN: JBSDD6; ISSN: 0739-1102  
 LANGUAGE: English  
 AB Numerous diseases have been linked to the malfunction of G-protein coupled receptors (GPCRs). Their adequate treatment requires rational design of new high-affinity and high-selectivity drugs targeting these receptors. The authors report three-dimensional models of the human MT1 and MT2 melatonin receptors, members of the GPCR family. The models are based on the x-ray structure of bovine rhodopsin. The computational approach employs an original procedure for optimization of receptor-ligand structures. It includes rotation of one of the transmembrane  $\alpha$ -helices around its axis with simultaneous assessment of the resulting complexes according to a number of criteria the authors

have developed for this purpose. The optimal geometry of the receptor-ligand binding is selected based on the anal. of complementarity of hydrophobic/hydrophilic properties between the ligand and its protein environment in the binding site. The elaborated "optimized" models are employed to explore the details of protein-ligand interactions for melatonin and a number of its analogs with known affinity to MT1 and MT2 receptors. The models permit rationalization of exptl. data, including those that were not used in model building. The perspectives opened by the constructed models and by the optimization procedure in the design of new drugs are discussed.

IT 244160-10-9  
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
 (three-dimensional models of human melatonin receptors MT1 and MT2 in relation to interactions with melatonin and analogs)  
 RN 244160-10-9 CAPLUS  
 CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)

L4 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



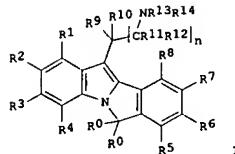
REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:2887 CAPLUS  
 DOCUMENT NUMBER: 140:77024  
 TITLE: Preparation of tetracyclic arylalkyl indoles having serotonin receptor affinity  
 INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambampati, Rama Satri; Battula, Srinivas Reddy; Rao, Venkata Satya Veerabhadra Vadlamudi  
 PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India  
 SOURCE: PCT Int. Appl., 66 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200400845	A1	20031231	WO 2003-IN224	20030619
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, NX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, RM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
IN 2002MA00476	A	20070518	IN 2002-MA476	20020621
CA 2490115	A1	20031231	CA 2003-2490115	20030619
AU 2003249584	A1	20040106	AU 2003-249584	20030619
BR 2003012175	A	20050405	BR 2003-12175	20030619
EP 1537113	A1	20050608	EP 2003-760959	20030619
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1662538	A	20050831	CN 2003-814597	20030619
JP 2006501175	T	20060112	JP 2004-515420	20030619
US 2005203103	A1	20050915	US 2005-518624	20050513
PRIORITY APPLN. INFO.:			IN 2002-MA476	A 20020621
		WO 2003-IN224		W 20030619

OTHER SOURCE(S): MARPAT 140:77024  
 GI

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The title compds. [I]: R0 = H, alkyl; R1-R12 = H, halo, oxo, thio, etc.; OR the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; n = 1-8; useful for treating conditions where a modulation of 5-HT and/or serotonin activity is desired [no data], were prepared. Thus, reacting 1-(2'-bromobenzyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl2(P(o-tolyl)3)2 and AcOK afforded 1-(2-N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indole. This invention also relates to processes for preparing the compds. I, compns. containing effective amts. of the compound I and the use of such a compound/composition in therapy.

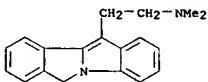
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 639809-42-0P 639809-44-2P 639809-46-4P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of isoindolo[2,1-a]indoles having serotonin receptor affinity)

RN 639808-61-0 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)

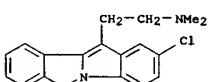
11/06/2007

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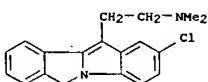
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-62-1 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl- (9CI)  
(CA INDEX NAME)



RN 639808-63-2 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



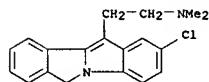
● x HCl

RN 639808-64-3 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 639808-62-1  
CMF C19 H19 Cl N2

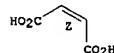
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 110-16-7  
CMF C4 H4 O4

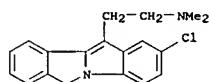
Double bond geometry as shown.



RN 639808-65-4 CAPLUS  
CN Butanedioic acid, hydroxy-, compd. with 2-chloro-N,N-dimethyl-6H-isindolo[2,1-a]indole-11-ethanamine (9CI) (CA INDEX NAME)

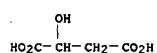
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CRN 639808-62-1  
CMF C19 H19 Cl N2



CM 2

CRN 6915-15-7  
CMF C4 H6 O5

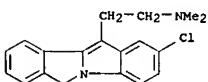


RN 639808-66-5 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-,

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

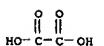
CM 1

CRN 639808-62-1  
CMF C19 H19 Cl N2



CM 2

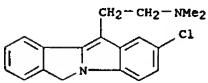
CRN 144-62-7  
CMF C2 H2 O4



RN 639808-67-6 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-chloro-N,N-dimethyl-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

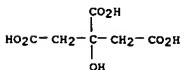
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CRN 639808-62-1  
CMF C19 H19 Cl N2



CM 2

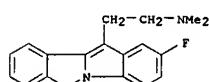
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CMF C6 H8 O7



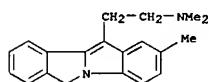
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L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

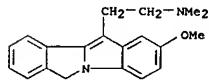
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CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-fluoro-N,N-dimethyl- (9CI)  
(CA INDEX NAME)



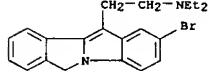
RN 639808-69-8 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, N,N,2-trimethyl- (9CI) (CA INDEX NAME)



RN 639808-70-1 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



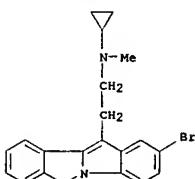
RN 639808-71-2 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-bromo-N,N-diethyl- (9CI) (CA INDEX NAME)



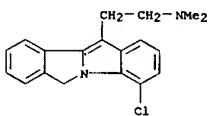
RN 639808-72-3 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-ethanamine, 2-bromo-N-cyclopropyl-N-methyl- (9CI) (CA INDEX NAME)

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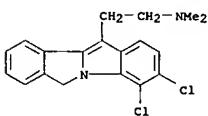
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-73-4 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-chloro-N,N-dimethyl- (9CI)  
(CA INDEX NAME)

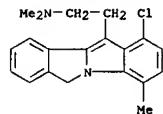


RN 639808-74-5 CAPLUS  
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(CA INDEX NAME)

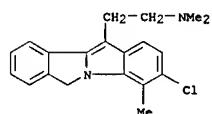


RN 639808-75-6 CAPLUS  
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(CA INDEX NAME)

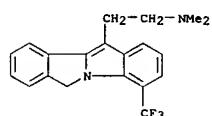
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-76-7 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,N,4-trimethyl- (9CI)  
(CA INDEX NAME)

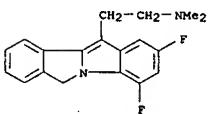


RN 639808-77-8 CAPLUS  
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(CA INDEX NAME)

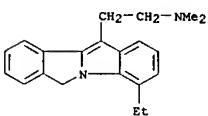


RN 639808-78-9 CAPLUS  
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(CA INDEX NAME)

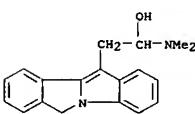
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



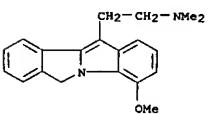
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(CA INDEX NAME)



RN 639808-86-9 CAPLUS  
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(CA INDEX NAME)

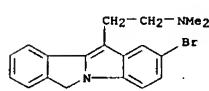


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(CA INDEX NAME)

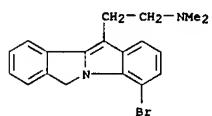


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(CA INDEX NAME)

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639808-89-2 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-bromo-N,N-dimethyl- (9CI)  
(CA INDEX NAME)



RN 639808-90-5 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 4-fluoro-N,N-dimethyl- (9CI)  
(CA INDEX NAME)



RN 639809-23-7 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 2-chloro-N-cyclopropyl-N-methyl-,  
2-hydroxy-1,2,3-propanetricarboxylate (9CI)  
(CA INDEX NAME)

CM 1

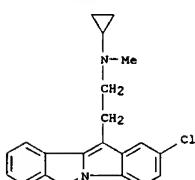
CRN 639809-22-6  
CMF C21 H21 Cl N2

11/06/2007

10518612

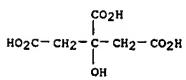
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

(Continued)

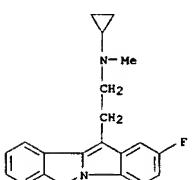


CM 2

CRN 77-92-9  
CNF C6 H8 O7

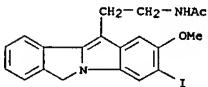


RN 639809-25-9 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, N-cyclopropyl-2-fluoro-N-methyl- (9CI) (CA INDEX NAME)

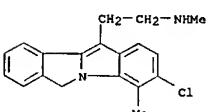


RN 639809-27-1 CAPLUS  
CN Acetamide, N-acetyl-N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

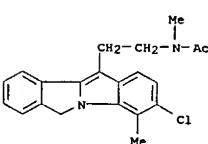
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
(9CI) (CA INDEX NAME)



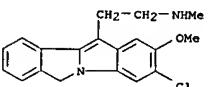
RN 639809-39-5 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-N,4-dimethyl- (9CI) (CA INDEX NAME)



RN 639809-41-9 CAPLUS  
CN Acetamide,  
N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-N-methyl- (9CI) (CA INDEX NAME)

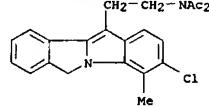


RN 639809-42-0 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-chloro-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)

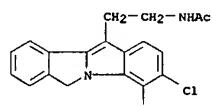


RN 639809-44-2 CAPLUS  
11/06/2007

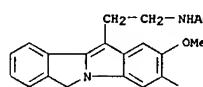
L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



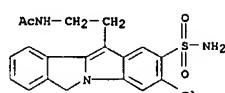
RN 639809-29-3 CAPLUS  
CN Acetamide, N-[2-(3-chloro-4-methyl-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639809-32-8 CAPLUS  
CN Acetamide,  
N-[2-(3-chloro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

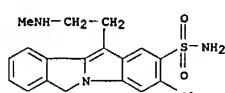


RN 639809-35-1 CAPLUS  
CN Acetamide, N-[2-(aminosulfonyl)-3-chloro-6H-isoindolo[2,1-a]indol-11-yl]ethyl- (9CI) (CA INDEX NAME)

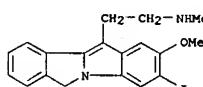


RN 639809-38-4 CAPLUS  
CN Acetamide, N-[2-(3-iodo-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]-

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639809-46-4 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-ethanamine, 3-iodo-2-methoxy-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10518612

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2004:2617 CAPLUS  
 DOCUMENT NUMBER: 140:77023  
 TITLE: Preparation of novel tetracyclic arylcarbonyl indoles having serotonin receptor affinity  
 INVENTOR(S): Jasti, Venkateswarlu; Ramakrishna, Venkata Satya Nirogi; Kambhampati, Rama Sastry; Battula, Srinivasa Reddy; Rao, Venkata Satya Veerabhadra Vadlamudi  
 PATENT ASSIGNEE(S): Suven Pharmaceuticals Ltd., India; Suven Life Sciences  
 Ltd.  
 SOURCE: PCT Int. Appl., 63 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200400205	A2	20031231	WO 2003-IN223	20030619
WO 200400205	A3	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, T2, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: BG, GM, KE, LS, MW, MZ, SD, SL, SZ, T2, UG, ZM, ZW, AM, AZ, BY, KG, K2, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
IN 2002MA0477	A	20060915	IN 2002-M4477	20020621
CA 2490002	A1	20031231	CA 2003-2490002	20030619
AU 2003249583	A1	20040106	AU 2003-249583	20030619
EP 1517909	A2	20050330	EP 2003-760858	20030619
EP 1517909	B1	20061025		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012174	A	20050405	BR 2003-12174	20030619
CN 1665815	A	20050907	CN 2003-814592	20030619
JP 2005537239	T	20051208	JP 2004-515419	20030619
AT 343580	T	20061115	AT 2003-760858	20030619
US 2005250834	A1	20051110	US 2005-518612	20050513
HK 1074630	A1	20070119	HK 2005-108744	20050930
PRIORITY APPLN. INFO.:			IN 2002-M4477	A 20020621
			WO 2003-IN223	W 20030619

OTHER SOURCE(S): MARPAT 140:77023  
 GI

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 639805-05-3 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

RN 639805-06-4 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)

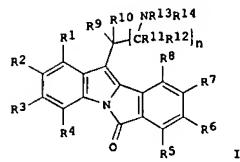
RN 639805-07-5 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

● HCl

RN 639805-05-3  
 CN 639805-05-3  
 CMF C19 H17 F N2 O

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L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



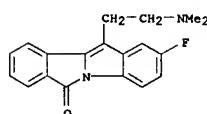
AB The title compds. [I; R1-R12 = H, halo, oxo, thio, etc.; or the adjacent groups like R1 and R2, etc. together with carbon atoms to which they are attached may form 5-7 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; or R9 and R10 or R11 and R12 together with the carbon atoms to which they are attached may form a 3-6 membered ring which may further contain one or more double bonds and/or one or more heteroatoms such as O, N, S or Se; R13 and R14 = H, alkyl, cycloalkyl, aryl, etc.; or NR13R14 = 3-7 membered heterocyclyl; 1 = 8], useful for treating conditions where the modulation of 5-HT and/or serotonin activity is desired (no data), were prepared Thus, reacting 1-(2'-bromobenzoyl)-N,N-dimethyltryptamine with N,N-dimethylacetamide in the presence of PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub>J and AcOK afforded 11-(2-(N,N-dimethylaminoethyl)-6H-isoindolo[2,1-a]indol-6-one. This invention also relates to processes for preparing the compds. I, compns. containing effective amts. of the compound I and the use of such a compound/composition in therapy.

IT 639805-04-2P 639805-05-3P 639805-06-4P  
 639805-07-5P 639805-08-6P 639805-09-7P  
 639805-10-0P 639805-11-1P 639805-12-2P  
 639805-13-3P 639805-14-4P 639805-15-5P  
 639805-16-6P 639805-17-7P 639805-18-8P  
 639805-19-9P 639805-20-2P 639805-21-3P  
 639805-22-4P 639805-24-6P 639805-25-7P  
 639805-26-8P 639805-27-9P 639805-28-0P  
 639805-51-9P 639805-52-0P 639805-53-1P  
 639805-54-2P 639805-55-3P 639805-56-4P  
 639805-57-5P 639805-58-6P 639805-59-7P  
 639805-60-0P 639805-61-1P 639805-62-2P  
 639805-63-3P 639805-64-4P

RL PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of isoindolo[2,1-a]indolones having serotonin receptor affinity)

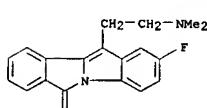
RN 639805-04-2 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2  
 CRN 110-16-7  
 CMF C4 H4 O4  
 Double bond geometry as shown.

CRN 639805-05-3  
 CMF C19 H17 F N2 O



CM 2  
 CRN 6915-15-7  
 CMF C4 H6 O5

OH  
 HO<sub>2</sub>C—CH—CH<sub>2</sub>—CO<sub>2</sub>H

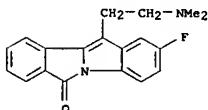
RN 639805-09-7 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-,

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L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
ethanediolate (9CI) (CA INDEX NAME)

CM 1

CRN 639805-05-3  
CMF C19 H17 F N2 O



CM 2

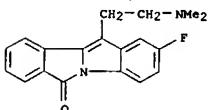
CRN 144-62-7  
CMF C2 H2 O4



RN 639805-10-0 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-fluoro-, 2-hydroxy-1,2,3-propanetricarboxylate (9CI) (CA INDEX NAME)

CM 1

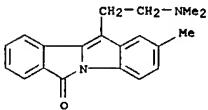
CRN 639805-05-3  
CMF C19 H17 F N2 O



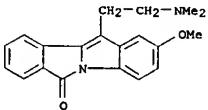
CM 2

CRN 77-92-9  
CMF C6 H8 O7

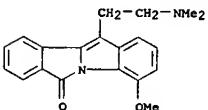
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
RN 639805-14-4 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methyl- (9CI) (CA INDEX NAME)



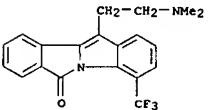
RN 639805-15-5 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2-methoxy- (9CI) (CA INDEX NAME)



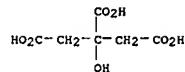
RN 639805-16-6 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-methoxy- (9CI) (CA INDEX NAME)



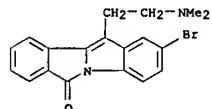
RN 639805-17-7 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



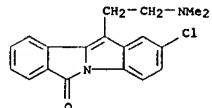
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



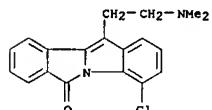
RN 639805-11-1 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-bromo-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-12-2 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 2-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

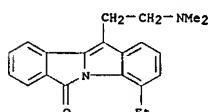


RN 639805-13-3 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 4-chloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

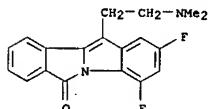


L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

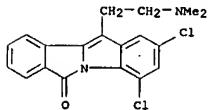
RN 639805-18-8 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-4-ethyl- (9CI) (CA INDEX NAME)



RN 639805-19-9 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-difluoro- (9CI) (CA INDEX NAME)



RN 639805-20-2 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 2,4-dichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

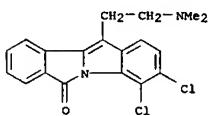


RN 639805-21-3 CAPLUS  
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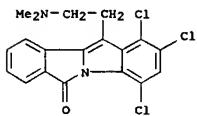
11/06/2007

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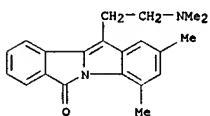
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



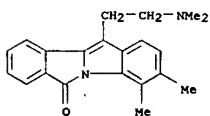
RN 639805-22-4 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 1,2,4-trichloro-11-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



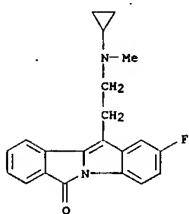
RN 639805-24-6 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-2,4-dimethyl- (9CI) (CA INDEX NAME)



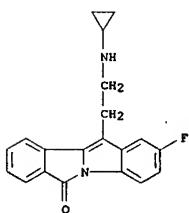
RN 639805-25-7 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(dimethylamino)ethyl]-3,4-dimethyl- (9CI) (CA INDEX NAME)



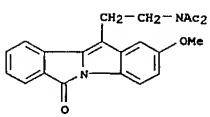
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639805-52-0 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 11-[2-(cyclopropylamino)ethyl]-2-fluoro- (9CI) (CA INDEX NAME)



RN 639805-53-1 CAPLUS  
CN Acetamide, N-acetyl-N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

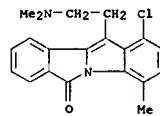


RN 639805-54-2 CAPLUS  
CN Acetamide, N-[2-(2-methoxy-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

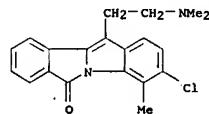
11/06/2007

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

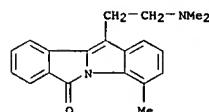
RN 639805-26-8 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 1-chloro-11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 639805-27-9 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-chloro-11-[2-(dimethylamino)ethyl]-4-methyl- (9CI) (CA INDEX NAME)

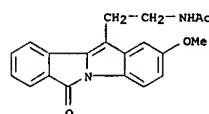


RN 639805-28-0 CAPLUS  
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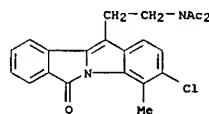


RN 639805-51-9 CAPLUS  
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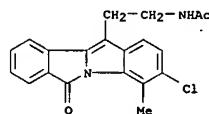
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



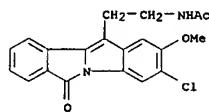
RN 639805-55-3 CAPLUS  
CN Acetamide,  
N-acetyl-N-[2-(3-chloro-4-methyl-6-oxo-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-56-4 CAPLUS  
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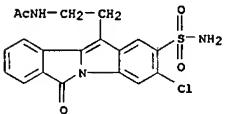
RN 639805-57-5 CAPLUS  
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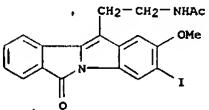
RN 639805-58-6 CAPLUS  
CN Acetamide,  
N-[2-(aminosulfonyl)-3-chloro-6-oxo-6H-isoindolo[2,1-a]indol-

10518612

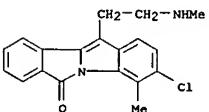
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
11-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 639805-59-7 CAPLUS  
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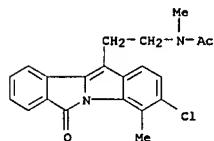


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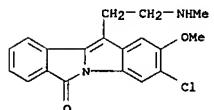


RN 639805-61-1 CAPLUS  
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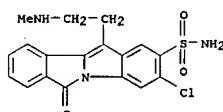
L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 639805-62-2 CAPLUS  
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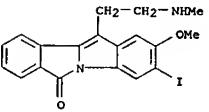


RN 639805-63-3 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-2-sulfonamide, 3-chloro-11-(2-(methylamino)ethyl)-6-oxo- (9CI) (CA INDEX NAME)



RN 639805-64-4 CAPLUS  
CN 6H-Isoindolo[2,1-a]indol-6-one, 3-iodo-2-methoxy-11-(2-(methylamino)ethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2003-215250 CAPLUS  
DOCUMENT NUMBER: 138:362155  
TITLE: Three-Dimensional Quantitative Structure-Activity Relationship Studies on Selected MT1 and MT2

Melatonin

Receptor Ligands: Requirements for Subtype

Selectivity and Intrinsic Activity Modulation  
AUTHOR(S): Rivara, Silvia; Mor, Marco; Silva, Claudia; Zuliani, Valentina; Vacondo, Federica; Spadoni, Gilberto; Bedini, Annalisa; Tarzia, Giorgio; Lucini, Valeria; Pannacci, Marilou; Fraschini, Franco; Plazzi, Pier Vincenzo

CORPORATE SOURCE: Dipartimento Farmaceutico, Universita degli Studi di Parma, Parma, I-43100, Italy

SOURCE: Journal of Medicinal Chemistry (2003), 46(8), 1429-1439

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The three-dimensional quant. structure-activity relation comparative mol. field anal. (3D-QSAR CoMFA) approach was applied to some classes of melatonin (MLT) membrane receptor ligands, with the principal aim of exploring the correlation between their steric features and MT2-selective antagonism. Binding data obtained from cloned MT1 and MT2 receptor subtypes were used to develop 3D-QSAR models for agonists and for antagonists at the two receptor subtypes, looking for the structural requirements for receptor subtype selectivity. In particular, we superposed the compds. showing antagonist activity, or very low intrinsic activity at the GTPyS test, following the hypothesis that the occupation of an addnl. pocket positioned out of the plane of MLT is one of the major determinants for MT2 selectivity; the statistical models obtained confirmed this hypothesis. Structure-intrinsic activity relation studies, applied to a set of compds. homogeneously tested, allowed the identification of the structural features whose modulation shifts the behavior from that of the agonist to that of the antagonist. The pocket out of the plane of MLT was identified as one of the key features for obtaining selective MT2 antagonists. The reliability of our statistical models was further confirmed by the correct prediction of the pharmacol. behavior of some N-substituted melatonin derivs., which were prepared and tested on cloned receptor subtypes.

IT 244160-10-9 263865-08-3 263865-09-4  
263865-11-8 263865-12-9 263865-13-0

263865-14-1 263865-15-2 263865-16-3

263865-17-4 263865-18-5 263865-19-6

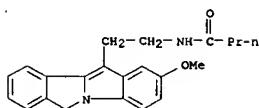
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(QSAR of MT1 and MT2 melatonin receptor ligands)

RN 244160-10-9 CAPLUS

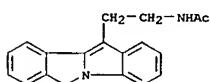
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)

10518612

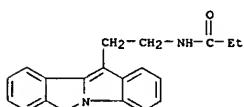
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-08-3 CAPLUS  
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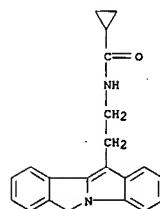


RN 263865-09-4 CAPLUS  
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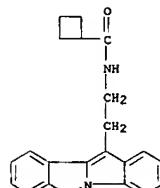


RN 263865-11-8 CAPLUS  
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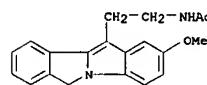
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-12-9 CAPLUS  
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

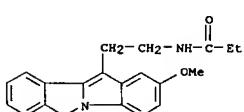


RN 263865-13-0 CAPLUS  
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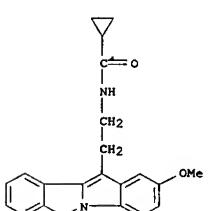


RN 263865-14-1 CAPLUS  
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI)

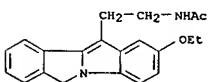
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-15-2 CAPLUS  
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

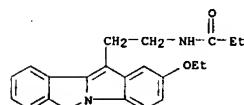


RN 263865-16-3 CAPLUS  
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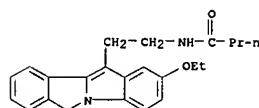


RN 263865-17-4 CAPLUS  
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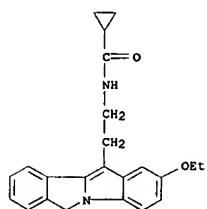
L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-18-5 CAPLUS  
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



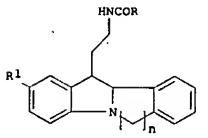
RN 263865-19-6 CAPLUS  
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: THIS 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10518612

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2002:974419 CAPLUS  
 DOCUMENT NUMBER: 138:395420  
 TITLE: 3D-QSAR analyses of melatonin antagonists  
 AUTHOR(S): Zhu, Li-Li; Xu, Xiao-Jie  
 CORPORATE SOURCE: College Chem. Molecular Eng., Peking Univ., Beijing,  
 100871, Peop. Rep. China  
 SOURCE: Wuli Huaxue Xuebao (2002), 18(12), 1087-1092  
 PUBLISHER: Beijing Daxue Chubanshe  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 GI

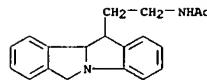


AB In this paper, two kinds of 3D-QSAR techniques: comparative mol. fields anal. (CoMFA) and comparative similarity indexes anal. (CoMSIA) were applied using a data set of 37 melatonin antagonists (I, R=alkyl or alicyclic; R<sup>1</sup>=H, Cl, or alkoxy; n=1-3). The influences of different grid spacing and partial charge models were systematically investigated. The CoMFA contour plots identified several essential features including steric and electrostatic fields, which are valuable for us to take insight into the mechanisms of the intermol. interactions between inhibitors and receptor.

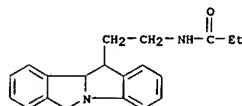
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 532394-18-8 532394-20-0 532394-21-1  
 532394-22-2 532394-24-4  
 RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)  
 (3D-QSAR analyses of melatonin antagonists)

RN 532394-07-3 CAPLUS  
 CN Acetamide, N-[2-(10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

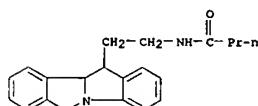
L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-08-4 CAPLUS  
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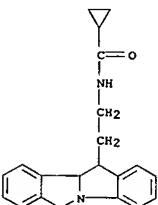


RN 532394-09-5 CAPLUS  
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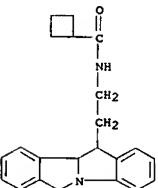


RN 532394-10-8 CAPLUS  
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L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-12-0 CAPLUS  
 CN Cyclobutanecarboxamide, N-[2-(10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

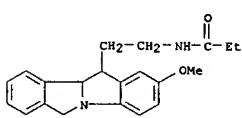


RN 532394-13-1 CAPLUS  
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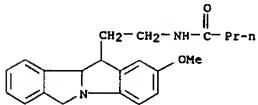


RN 532394-14-2 CAPLUS  
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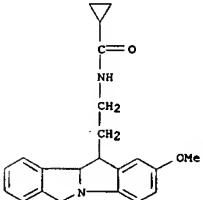
L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-15-3 CAPLUS  
 CN Butanamide, N-[2-(10b,11-dihydro-2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



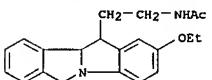
RN 532394-16-4 CAPLUS  
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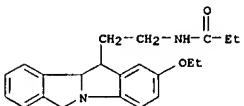
RN 532394-18-6 CAPLUS  
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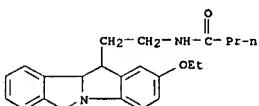
L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-20-0 CAPLUS  
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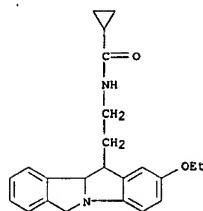


RN 532394-21-1 CAPLUS  
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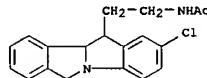


RN 532394-22-2 CAPLUS  
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L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 532394-24-4 CAPLUS  
CN Acetamide, N-[2-(2-chloro-10b,11-dihydro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 200210274 CAPLUS  
DOCUMENT NUMBER: 136:64149

TITLE: 6H-Isoindolo[2,1-a]indoles or 5,6-dihydroisoindolo[2,1-a]isoquinolines as subtype-selective melatonergics for therapeutic use

INVENTOR(S): Jones, Robert M.

PATENT ASSIGNEE(S): Cognitix, Inc., USA

SOURCE: PCT Int. Appl., 40 pp.

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200200215	A1	20020103	WO 2001-US19959	20010622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZR, ZS, ZT, ZU, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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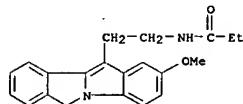
OTHER SOURCE(S): MARPAT 136:64149

AB The invention disclosed the use of MT2 selective melatonergics as anticonvulsant agents and as analgesic agents. More specifically, the invention disclosed the use of 6H-isocindolo[2,1-a]indoles or 5,6-dihydroisocindolo[2,1-a]isoquinolines which have melatonin agonist activity and which are selective for the MT2 receptor as anticonvulsant agents or analgesic agents. The invention further relates to the use of 5,6-dihydroisocindolo[2,1-a]isoquinolines and 6,7-dihydro-5H-benzodiazepino[2,1-a]indoles which have melatonin antagonist activity and which are selective for the MT2 receptor as pharmacol. tools for delineation of physiol. responses governed by MT2 receptor activation either by melatonin or selective agonists disclosed herein and for treatment of disorders associated with overprodn. of melatonin such as seasonal affective disorder (SAD) and shift work syndrome. Such melatonin antagonists are also useful for treating Parkinson's Disease.

IT 263865-14-1, CGX 031-120  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(isocindoloindole derivs. and dihydroisocindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)

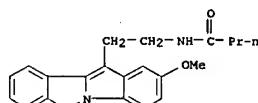
RN 263865-14-1 CAPLUS  
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

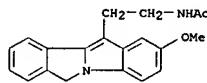


IT 244160-10-9, CGX 031139 263865-13-0, CGX 031133  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(phenacyclidine-like behavior; isoindoloindole derivs. and dihydroisocindoloisoquinoline derivs. as subtype-selective melatonergics for therapeutic use)

RN 244160-10-9 CAPLUS  
CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



RN 263865-13-0 CAPLUS  
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

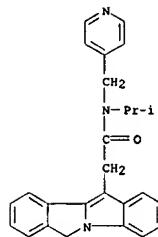


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10518612

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2001:246308 CAPLUS  
 DOCUMENT NUMBER: 135:70637  
 TITLE: 2-Arylindole-3-acetamides FPP-Competitive inhibitors  
 of farnesyl protein transferase  
 AUTHOR(S): Trotter, B. W.; Quigley, A. G.; Lumma, W. C.; Sisko, J. T.; Walsh, E. S.; Hamann, C. S.; Robinson, R. G.; Bhimnathwala, H.; Kolodin, D. G.; Zheng, W.; Buser, C.  
 A.: Huber, H. E.; Lobell, R. B.; Kohl, N. E.; Williams, T. M.; Graham, S. L.; Dinsmore, C. J.  
 CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2001), 11(7), 865-869  
 CODEN: BMCLB; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A series of 2-arylindole-3-acetamide farnesyl protein transferase inhibitors has been identified. The compds. inhibit the enzyme in a farnesyl pyrophosphate-competitive manner and are selective for farnesyl protein transferase over the related enzyme geranylgeranyltransferase-I.  
 A representative member of this series of inhibitors demonstrates equal effectiveness against HDJ-2 and K-Ras farnesylation in a cell-based assay when geranylgerylation is suppressed.  
 IT 347373-82-4P  
 RL: BRC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (arylindole acetamides farnesyl pyrophosphate-competitive inhibitors of farnesyl protein transferase)  
 RN 347373-82-4 CAPLUS  
 CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N-(1-methylethyl)-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

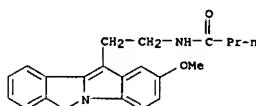
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2000:185117 CAPLUS  
 DOCUMENT NUMBER: 132:273842  
 TITLE: Mapping the Melatonin Receptor. 6. Melatonin Agonists and Antagonists Derived from 6H-Isoindolo[2,1-a]indoles, 5,6-Dihydroisoindolo[2,1-a]isoquinolines, and 6,7-Dihydro-5H-benzoc[c]azepino[2,1-a]indoles  
 AUTHOR(S): Faust, Ruediger; Garratt, Peter J.; Jones, Rob; Yeh, Li-Kuan; Tsotinis, Andrew; Panoussopoulou, Maria; Calogeropoulou, Theodora; Teh, May-Teck; Sugden, David  
 CORPORATE SOURCE: Department of Chemistry, University College London, London, WC1H 0AJ, UK  
 SOURCE: Journal of Medicinal Chemistry (2000), 43(6), 1050-1061  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 6H-Isoindolo[2,1-a]indoles, 5,6-dihydroisoindolo[2,1-a]isoquinolines, and 6,7-dihydro-5H-benzoc[c]azepino[2,1-a]indoles have been prepared as melatonin analogs to investigate the nature of the binding site of the melatonin receptor. The affinity of analogs was determined in a radioligand binding assay using cloned human m1 and MT2 receptor subtypes expressed in NIH 3T3 cells. Agonist and antagonist potency was measured using the pigment aggregation response of a clonal line of Xenopus laevis melanophores. The 2-methoxyisoindolo[2,1-a]indoles showed much higher binding affinities than the parent isoindoles and whereas 2-methoxyisoindolo[2,1-a]indoles were agonists in the functional assay, its cyclopropanecarbonyl derivative and parent isoindoles were antagonists. The 2-ethoxyisoindolo[2,1-a]indoles showed reduced binding affinities compared to their methoxy analogs, while the 5-chloro derivative showed a considerable reduction in binding affinity and potency compared to acetyl 2-methoxyisoindolo[2,1-a]indole compound. The 10-methoxy-5,6-dihydroisoindolo[2,1-a]isoquinolines had higher binding affinities than the corresponding parent indoloisoquinolines in the human receptor subtypes, and the parent compds. were antagonists, whereas the 10-methoxy derivs. were agonists in the functional assay. The N-cyclobutanecarbonyl derivs. of both the parent and 10-methoxy series had similar binding affinities and were both antagonists with similar potencies. The 11-methoxy-6,7-5H-benzoc[c]azepino[2,1-a]indoles had higher binding affinities than the corresponding parent compds. at the MT2 receptor but similar affinities at the m1 site; all of the compds. were antagonists in the functional assay. Changing 11-methoxy for 11-ethoxy decreased the binding affinity slightly, and this was more evident at the MT2 receptor. All of the derivs. investigated had either the same or a greater affinity for the human MT2 receptor compared to the m1 receptor (range 1:1-1:32). This suggests that the m1 and MT2 receptor pockets differ in their ability to accommodate alkyl groups in the indole nitrogen region of the melatonin mol. Two compds. were tested in functional assays on recombinant m1 and MT2 melatonin receptors. N-butanoyle 2-(9-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethanamine was a potent

L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 agonist with some selectivity (44-fold) for the MT2 receptor, while N-butanoyle 2-(5,6,7-trihydro-11-methoxybenzo[c]cyclohept[2,1-a]indol-13-yl)ethanamine was an MT2-prefering antagonist. Increasing the carbon chain length between N-1 of indole and the 2-Ph group from n = 1 through

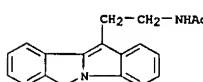
n = 3 leads to a fairly regular decrease in the binding affinity, but, remarkably, when n = 3, it converts the methoxy compds. from melatonin agonists to antagonists. The Xenopus melatonin receptor thus cannot accommodate an N-n-alkyl chain attached to a 2-Ph substituent with n > 2 in the required orientation to induce or stabilize the active receptor conformation.

IT 244160-10-9P 263865-08-3P 263865-09-4P  
 263865-10-7P 263865-11-8P 263865-12-9P  
 263865-13-0P 263865-14-1P 263865-15-2P  
 263865-16-3P 263865-17-4P 263865-18-5P  
 263865-19-6P 263865-20-9P  
 RL: BRC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation and structure of melatonin agonists and antagonists derived from isoindoloindoless, indoloisoquinolines, and benzoazepinoindoless)

RN 244160-10-9 CAPLUS  
 CN Butanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



RN 263865-08-3 CAPLUS  
 CN Acetamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

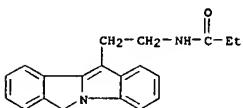


RN 263865-09-4 CAPLUS  
 CN Propanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

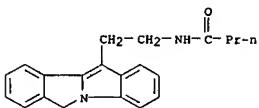
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L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN

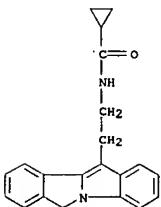
(Continued)



RN 263865-10-7 CAPLUS  
CN Butanamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

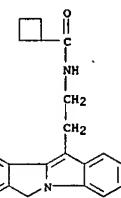


RN 263865-11-8 CAPLUS  
CN Cyclopropanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

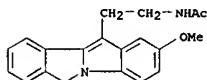


RN 263865-12-9 CAPLUS  
CN Cyclobutanecarboxamide, N-[2-(6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

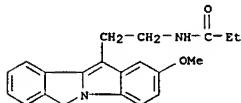
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-13-0 CAPLUS  
CN Acetamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

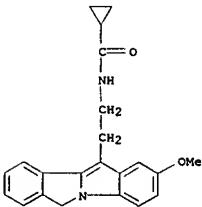


RN 263865-14-1 CAPLUS  
CN Propanamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

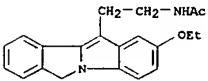


RN 263865-15-2 CAPLUS  
CN Cyclopropanecarboxamide, N-[2-(2-methoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

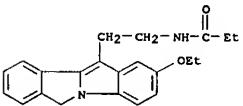
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-16-3 CAPLUS  
CN Acetamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

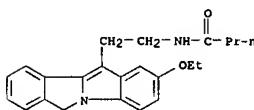


RN 263865-17-4 CAPLUS  
CN Propanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

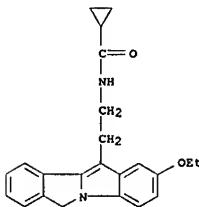


RN 263865-18-5 CAPLUS  
CN Butanamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)

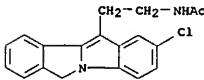
L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 263865-19-6 CAPLUS  
CN Cyclopropanecarboxamide, N-[2-(2-ethoxy-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



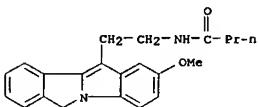
RN 263865-20-9 CAPLUS  
CN Acetamide, N-[2-(2-chloro-6H-isoindolo[2,1-a]indol-11-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: THIS THERE ARE 58 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10518612

L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1995:442966 CAPLUS  
DOCUMENT NUMBER: 131:240681  
TITLE: Design of subtype selective melatonin receptor agonists and antagonists  
AUTHOR(S): Sugden, David; Yeh, Li-Kuan; Teh, Muy-Teck  
CORPORATE SOURCE: Physiology Division, GKT School of Biomedical Science,  
SOURCE: King's College London, London, W8 7AH, UK  
PUBLISHER: Reproduction, Nutrition, Development (1999), 39(3), 335-344  
DOCUMENT TYPE: CODEN: RNDEES; ISSN: 0926-5287  
LANGUAGE: Editions Scientifiques et Medicales Elsevier  
Journal English  
AB Studies of the physiol. actions of melatonin have been hindered by the lack of specific, potent and subtype selective agonists and antagonists. We describe the utility of a melanophore cell line from *Xenopus laevis* for exploring structure-activity relationships among novel melatonin analogs and report a novel MT2-selective agonist (IIK7) and MT2-selective antagonist (K185). IIK7 is a potent melatonin receptor agonist in the melanophore model, and in NIH3T3 cells expressing human mtl and MT2 Receptor subtypes. In radioligand binding expts. IIK7 is 90-fold selective for the MT2 subtype. K185 is devoid of agonist activity, but acts as a competitive melatonin antagonist in melanophores. A low concentration (10-9M) antagonizes melatonin inhibition of forskolin stimulation of cAMP in NIH3T3 cells expressing human MT2 receptors, but has no effect in cells expressing mtl receptors. In binding assays, K185 is 140-fold selective for the MT2 subtype.  
IT 244160-10-9  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (melatonin analogs structure-activity relationship in frog melanophore and human melatonin receptors)  
RN 244160-10-9 CAPLUS  
CN Butanamide, N-[2-(2-methoxy-6H-isindolo[2,1-a]indol-11-yl)ethyl]- (CA INDEX NAME)



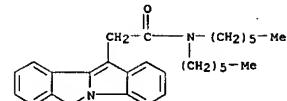
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993:662000 CAPLUS  
DOCUMENT NUMBER: 119:262000  
TITLE: Chemistry, binding affinities, and behavioral properties of a new class of "antineophobic" mitochondrial DBI receptor complex (mDRC) ligands  
AUTHOR(S): Kozikowski, A. P.; Ma, D.; Brewer, James; Sun, S.; Costa, E.; Romeo, E.; Guidotti, A.  
CORPORATE SOURCE: Mayo Found. Med. Educ. Res., Jacksonville, FL, 32224, USA  
SOURCE: Journal of Medicinal Chemistry (1993), 36(20), 2908-20  
DOCUMENT TYPE: CODEN: JMCMAR; ISSN: 0022-2623  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 119:262000  
AB The mitochondrial DBI (diazepam-binding inhibitor) receptor complex (mDRC; previously called the peripheral benzodiazepine receptors) is linked to the production of neurosteroids such as pregnenolone sulfate, dehydroepiandrosterone sulfate, and others. In order to gain further information as to the function of the mDRC in the brain, the authors have constructed and tested, both *in vitro* and *in vivo*, a novel series of ligands, 2-arylidole-3-acetamides. The SAR studies detailed herein delineate some of the structural features required for high affinity binding to the mDRCs. In most cases the new ligands were prepared by use of the Fischer indole synthesis. Variations in the length and number of the alkyl groups on the amide nitrogen were probed together with the effects of halogen substituents on one or both of the aryl rings. Some ligands were also synthesized for study which represent conformationally constrained versions of the parent structure. Broad screening studies revealed these indoleacetamides to be highly selective for the mDRC, since they failed to bind with any significant affinity to other receptor systems. Some of the ligands were found to exhibit Ki values in the low nanomolar range for the mDRC as measured by the displacement of [<sup>3</sup>H]4'-chlorodiazepam. A subset of these ligands was also shown to stimulate pregnenolone formation from the mitochondria of C6-2B glioma cells with an EC<sub>50</sub> of about 3 nM. In animal expts. ligands selected for further study were found to exhibit antineophobic effects, in spite of the fact that they exhibit no direct action on GABA<sub>A</sub> receptors.

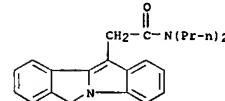
Consequently, it is postulated that these ligands owe their action to an indirect modulation of GABA<sub>A</sub> receptor function, presumably by stimulation of neurosteroid production and release from glial cells, followed by neurosteroid modulation of GABA<sub>A</sub>'s action on the chloride ion channel conductance of GABA<sub>A</sub> receptors.  
IT 147375-21-19  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABA<sub>A</sub> receptor function modulation and antineophobic activity in relation to)  
RN 147375-21-1 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 135966-96-0  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and mitochondrial diazepam-binding receptor complex affinity of, glial neurosteroid release and GABA<sub>A</sub> receptor function modulation and antineophobic activity in relation to)  
RN 135966-96-0 CAPLUS  
CN 6H-Isindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)

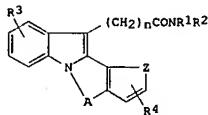


10518612

L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1993:233880 CAPLUS  
DOCUMENT NUMBER: 118:233880  
TITLE: Preparation of indolecarboxamides and methods of treating neurological and psychiatric disorders  
INVENTOR(S): Costa, Erminio; Guidotti, Alessandro; Kozikowski, Alan; Ma, Dawei  
PATENT ASSIGNEE(S): Fidia - Georgetown Institute for the Neurosciences, USA  
SOURCE: PCT Int. Appl., 55 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9300334	A1	19930107	WO 1992-US5246	19920626
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, PL, RO, RU, SD, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
US 5206382	A	19930427	US 1991-722196	19910627
AU 9222939	A	19930125	AU 1992-22939	19920626
EP 546164	A1	19930616	EP 1992-914902	19920626
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06501030	T	19940127	JP 1993-501593	19920626
PRIORITY APPLN. INFO.:			US 1991-722196	A 19910627
		WO 1992-US5246		A 19920626

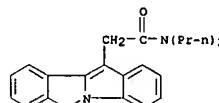
OTHER SOURCE(S): MARPAT 118:233880  
GI



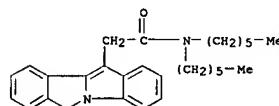
I

AB Title compds. I (R1, R2 = H, C3-12 alkyl, (alkyl)aryl; R1R2 = 4-6-membered (un)saturated ring; R3, R4 = H, C1-12 alkyl, O2N, H2N, N3, cyano, halo, RO2C, RO, RS (wherein R = H, alkyl); A = C1-3 alkylene to form a ring or null; Z = O, NH, S, CH:CH; n = 1-3) or their salts are prepared PhNNNH2, PhCOCH2CH2CO2H and H2SO4 in EtOH were refluxed for 24 h, cooled and extracted

L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
With Et2O to give Et 2-phenyl-3-indoleacetate which in 3N NaOH was refluxed for 3 h, acidified with HCl and treated with Me(CH2)5NH2, PhOP(O)(CH2)5NH2, and Et3N to give I (A = null, Z = CH:CH, R1 = R3 = R4 = H, R2 = hexyl, n = 1). I showed anxiolytic action in rodents at 0.1-0.5 mg/kg.  
IT 135966-96-0P 147375-21-1P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as drug for treatment of neurol. disorders and as antipsychotics)  
RN 135966-96-0 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



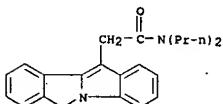
RN 147375-21-1 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dihexyl- (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 1991:535868 CAPLUS  
DOCUMENT NUMBER: 115:135868  
TITLE: Palladium catalyzed synthesis of annelated indoles  
AUTHOR(S): Kozikowski, Alan P.; Ma, Dawei  
CORPORATE SOURCE: Mayo Clin., Jacksonville, FL, 32224.. USA  
SOURCE: Tetrahedron Letters (1991), 32(28), 3317-20  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 115:135868  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The synthesis of polycyclic indoles, e.g., I (X = O, CH2), II, III, is shown to be accomplished readily by the palladium catalyzed intramol. cyclization of bromoarylindoles, e.g., IV, V, VI.  
IT 135966-96-0P  
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
RN 135966-96-0 CAPLUS  
CN 6H-Isoindolo[2,1-a]indole-11-acetamide, N,N-dipropyl- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST

63.71	236.02
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
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CA SUBSCRIBER PRICE

-9.36	-9.36
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